

Metastability, Nucleation, and Noise-Enhanced Stabilization Out of Equilibrium

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We study metastability and nucleation in a kinetic 2D-Ising model which is driven out of equilibrium by a small random perturbation of the usual dynamics at temperature T . We show that, at a mesoscopic/cluster level, a nonequilibrium potential describes in a simple way metastable states and their decay. We thus predict noise-enhanced stability of the metastable phase and resonant propagation of domain walls at low- T . This follows from the nonlinear interplay between thermal and nonequilibrium fluctuations, which induces reentrant behavior of the *surface tension* as a function of T . Our results, which are confirmed by Monte Carlo simulations, can be also understood in terms of a Langevin equation with competing additive and multiplicative noises.

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Relaxation in many natural systems proceeds through metastable states [1, 2, 3, 4, 5, 6, 7, 8, 9]. This is often observed in condensed matter physics [5], and also in various other fields, from cosmology [6] to biology [7] and high-energy physics [8]. In spite of such ubiquity, the microscopic understanding of metastability still raises fundamental questions. A main difficulty is that this is a dynamic phenomenon not included in the ensemble formalism. Even so, metastable states may be regarded in many cases as equilibrium states for times short compared with their relaxation time, and one may derive macroscopic properties from *restricted ensembles* [1], or obtain fluctuation-dissipation theorems [9]. On the long run, however, metastable states eventually decay triggered by rare fluctuations. This relaxation can be described in terms of free-energy differences as far as one is dealing with systems evolving towards equilibrium steady states [3]. However, as a rule, natural systems are open to the environment, which induces currents of macroscopic observables or competitions between opposing tendencies which typically break detailed balance [10]. Consequently, in many cases, stationary states are not equilibrium states, but are strongly influenced by dynamics, which adds further challenge to the microscopic understanding of metastability.

In this paper we report on the nature of metastability in a full nonequilibrium setting. In order to focus on the basic physics, we study the simplest nonequilibrium model in which metastable states are relevant, namely an Ising model with dynamic impurities. We show that introducing a nonequilibrium condition has dramatical effects on metastable dynamics. In particular, we find noise-enhanced stabilization of metastable states, resonant propagation of domain walls and other novel low temperature physics not observed in equilibrium. Surprisingly, these nonequilibrium phenomena can be understood via extended nucleation theory, starting

from a nonequilibrium potential or *free-energy* at a mesoscopic/cluster level. This is possible because the excitations responsible for the metastable-stable transition result from the competition between a surface and a bulk term, as in equilibrium. We thus anticipate that a similar approach can be used to understand metastability in many other nonequilibrium systems in which a surface/bulk competition is a dominant mechanism. Our results are also relevant for metastable nanodevices where nonequilibrium impurities play a fundamental role [10].

Consider a two-dimensional square lattice of side L with periodic boundary conditions. We define a spin variable $s_i = \pm 1$ at each node, $i \in [1, N \equiv L^2]$. Spins interact among them and with an external magnetic field h via the Ising Hamiltonian function, $\mathcal{H} = -\sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$, where the first sum runs over all nearest-neighbors pairs. We also define a stochastic single spin-flip dynamics with transition rate

$$\omega(\mathbf{s} \rightarrow \mathbf{s}^i) = p + (1-p)\Psi(\beta\Delta\mathcal{H}_i), \quad (1)$$

where $\mathbf{s} = \{s_k\}$ and \mathbf{s}^i stand for the configurations before and after flipping the spin at node i , respectively, $\Delta\mathcal{H}_i$ is the *energy* increment in such flip, and $\beta = 1/T$. The function in (1) is chosen here as $\Psi(x) = (1+e^x)^{-1}$, which corresponds to the *Glauber rate*. However, similar results hold also for the *Metropolis rate*, and possibly for many other local, detailed-balanced dynamical rules Ψ .

For any $0 < p < 1$ two different heat baths compete in (1): One is at temperature T , which operates with probability $(1-p)$, and the other induces completely random spin-flips (as a bath at *infinite* temperature would do) with probability p . As a result of this competition, a *nonequilibrium* steady state sets in asymptotically [10, 11, 12, 13], which cannot be characterized by any Gibbsian measure. For $h = 0$, the model exhibits an order-disorder continuous phase transition at temperature $T_c(p) < T_c(p=0) \equiv T_{\text{ons}}$, where

$T_{\text{ons}} = 2/\ln(1 + \sqrt{2})$, and the order washes out for any $p > p_c = (\sqrt{2} - 1)^2 \approx 0.17$, even at $T = 0$. This phase transition belongs to the Ising universality class, a result that has led to the belief that two-temperature nonequilibrium Ising models behave in general as their equilibrium ($p = 0$) counterpart. We show below that, in what concerns metastability, essential differences indeed exist.

We remark that our motivation here for the random perturbation p is that it is the simplest microscopic mechanism that induces nonequilibrium behavior. However, similar dynamic impurities play a fundamental role in some natural systems. As a matter of fact, an equivalent mechanism has been used to model the macroscopic consequences of rapidly-diffusing local defects [10] and quantum tunneling [11] in magnetic samples and, more generally, the origin of scale-invariant avalanches [14].

For small $h < 0$ and $T < T_c(p)$, an initial homogeneous state with all spins up is metastable. It will eventually decay toward the stable state of magnetization $m = N^{-1} \sum_i s_i < 0$. Inspection of escape configurations (Fig. 1) shows that this is a highly inhomogeneous process triggered by (large) compact clusters of the stable phase. These excitations then grow or shrink in the metastable sea depending on the competition between their surface, which hampers cluster growth, and their bulk, which favors it. In equilibrium ($p = 0$), this competition is controlled by the cluster interfacial free-energy, or surface tension. Far from equilibrium ($0 < p < 1$), despite the lack of a proper bulk free-energy function, one may define [13] an effective *surface tension* $\sigma_0(T, p)$, that captures the properties of the nonequilibrium interface. This is based on the assumption that the normalization of a probability measure for interface configurations can be interpreted as a sort of nonequilibrium *partition function*

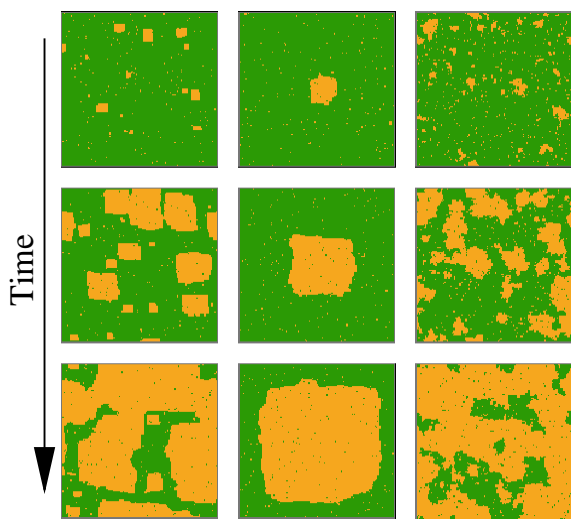


FIG. 1: (Color online) Escape configurations for $L = 128$, $p = 0.01$, $h = -0.25$ and $T/T_{\text{ons}} = 0.1, 0.3$ and 0.7 , respectively from left to right.

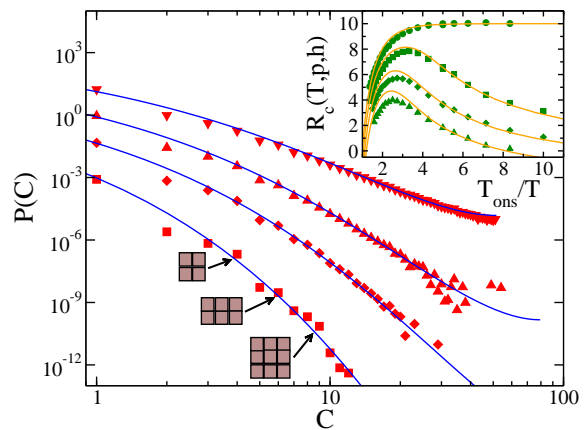


FIG. 2: (Color online) Cluster distribution $P(C)$ for $T = 0.2T_{\text{ons}}$, $L = 53$, $h = -0.1$ and, from bottom to top, $p = 0.001, 0.005, 0.01, 0.02$, with $\gamma = 0.815, 0.82, 0.83, 0.85$, respectively. Lines are theoretical predictions and points are MC results. Inset: \mathcal{R}_c vs. T_{ons}/T for $L = 53$, $h = -0.1$ and, from top to bottom, $p = 0, 0.001, 0.005$ and 0.01 . The n^{th} curve (from bottom to top) has been rescaled by a factor $10^{(n-1)}$ (main plot), or shifted $(4 - n)$ units (inset) in the \hat{y} -axis.

[13]. Similar assumptions have been shown to yield excellent results for nonequilibrium phase transitions [15]. Interesting enough, $\sigma_0(T, p)$ exhibits non-monotonous temperature dependence for any $0 < p < 1$ with a maximum at a non-trivial value of T [13, 16].

Consequently with the surface/bulk competition driving the relevant excitations, it is straightforward to write down an ansatz for an effective *free-energy* cost of a cluster of radius R , $\mathcal{F}(R) = \gamma[2\Omega R\sigma_0 - \Omega R^2 2m_0|h|]$; see [3, 4]. We may then derive the zero-field spontaneous magnetization $m_0(T, p)$ within a mean-field approximation [12] and the cluster form factor $\Omega(T, p)$ from σ_0 via the Wulff construction [13]; γ is a weakly-varying parameter, very close to one, that stands for small corrections to classical nucleation theory [4]. The critical cluster radius, such that supercritical (subcritical) clusters tend to grow (shrink), thus follows as $\mathcal{R}_c = \sigma_0/(2m_0|h|)$. Estimates of \mathcal{R}_c in MC simulations (see [17] for details) are shown in the inset to Fig. 2 together with the analytical predictions. The agreement is excellent for temperatures well below $T_c(p)$ and, most important, $\mathcal{R}_c(T, p, h)$ exhibits non-monotonous T -dependence for any $p > 0$.

Our ansatz above also implies a Boltzmann-like distribution, $P(C) = \mathcal{M}^{-1} \exp[-\beta\mathcal{F}(\sqrt{C/\Omega})]$ for the fraction of stable-phase clusters of volume $C = \Omega R^2$ in the metastable phase. The normalization $\mathcal{M} = 2\Theta/(1 - m)$, with $\Theta = \sum_{C=1}^{C_*} C \exp[-\beta\mathcal{F}(\sqrt{C/\Omega})]$ and $C_* = \Omega \mathcal{R}_c^2$, is defined so that the metastable state has the mean-field magnetization $m(T, p, h)$ [12]. Fig. 2 depicts our results for $P(C)$. Again, theoretical predictions compare very well to MC results. For $p = 0.001$, MC data reveal a non-trivial structure in $P(C)$ which is not captured by

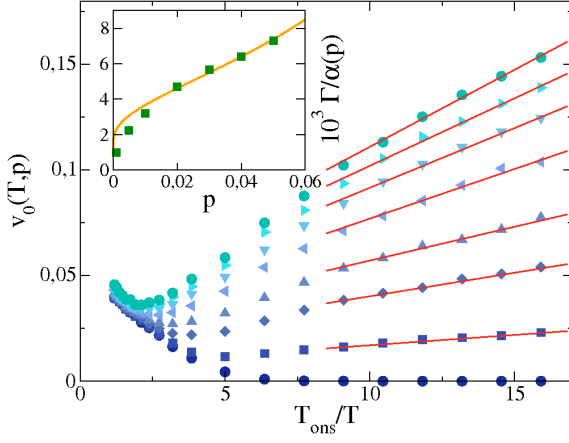


FIG. 3: (Color online) v_0 vs. T_{ons}/T for $h = -0.1$ and $p = 0, 0.001, 0.005, 0.01, 0.02, 0.03, 0.04, 0.05$ (from bottom to top). Curves are linear fits to data. Inset: Slope of linear fits vs. p . The line is the theoretical prediction, with $\Gamma \approx 0.0077$.

our continuous theory. This is due to the lattice structure which, for low- T and small p , gives rise to resonances for clusters with complete *shells*, i.e. 2×2 , 3×2 , 3×3 ; see Fig. 2. For larger p and/or T , fluctuations wash out this effect. Also interesting in Fig. 2 is that the nonequilibrium perturbation p enhances fluctuations and favors larger clusters.

The assumed $\mathcal{F}(R)$ also involves a force per unit area which controls the growth of supercritical droplets. In particular, the propagation velocity of a large cluster should obey the Allen-Cahn expression $v_0 = 2\Gamma m_0 |h|/\sigma_0$ [2], where Γ is a non-universal constant. Our estimates for v_0 in MC simulations of a flat propagating interface (an infinitely-large cluster) [17] are in Fig. 3. The fact that v_0 exhibits the expected non-monotonous T -dependence means that cooling the system favors domain wall propagation in a nonequilibrium setting. Moreover, $\sigma_0 \approx \alpha(p)T$ at low- T , with $\alpha(p) = \ln[(1 - \sqrt{p})/(p + \sqrt{p})]$ [13, 16, 17], so that we expect $v_0 \approx [\Gamma/\alpha(p)](T_{\text{ons}}/T)$ in this regime, where Γ is a different non-universal constant and we assumed $m_0(T \rightarrow 0, p) \approx 1$. This is nicely confirmed in simulations, see inset to Fig. 3.

The nucleation rate \mathcal{I} for critical clusters determines the metastable-state lifetime. From our hypothesis, $\mathcal{I} = A|h|^\delta \exp[-\beta\mathcal{F}(\mathcal{R}_c)]$, where $A(p)$ is a non-universal amplitude and $\delta \approx 3$ for random updatings [3]. The relaxation pattern depends on the balance between two different length scales, namely, L and the mean cluster separation $\mathcal{R}_0(T, p, h) = (v_0/\mathcal{I})^{1/3}$ (typically, $\mathcal{R}_c \ll \mathcal{R}_0, L$). For $\mathcal{R}_0 \gg L$ [Single-Droplet (SD) regime], nucleation of a *single* critical cluster is the relevant excitation, and the metastable-state lifetime is $\tau_{\text{SD}} = (L^2\mathcal{I})^{-1}$. For $\mathcal{R}_0 \ll L$ [Multidroplet (MD) regime], the metastable-state transition proceeds via the nucleation of many critical clusters, and $\tau_{\text{MD}} = [\Omega v_0^2 \mathcal{I}/(3 \ln 2)]^{-1/3}$ [3]. The crossover corresponds to the dynamic spinodal point,

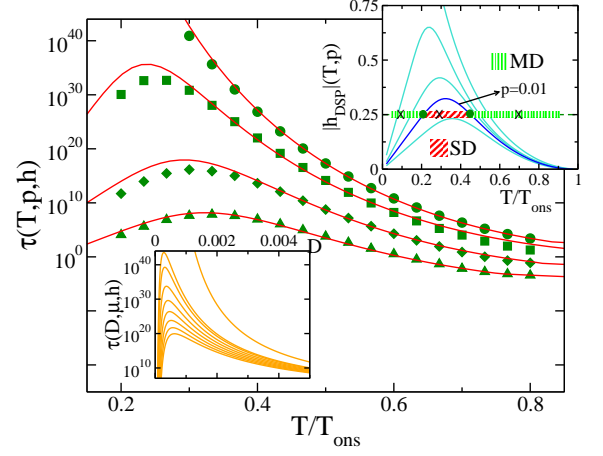


FIG. 4: (Color online) Lifetime τ vs. T for the same p and conditions than for the inset in Fig. 2. The n^{th} curve (from top to bottom) is rescaled by a factor $10^{-2(n-1)}$. Solid lines are theoretical predictions for (from top to bottom) $\gamma = 1, 0.85, 0.77, 0.65$. Amplitudes $A(p) \in [10^{-3}, 10^{-2}]$. Top inset: $|h_{\text{DSP}}|$ vs. T for (from top to bottom) $p = 0, 0.001, 0.005, 0.01, 0.02$. Bottom inset: τ vs. D , as derived from Langevin equation, for $h = -0.1$ and $\mu \in [0, 6 \times 10^{-3}]$, increasing from top to bottom.

$|h_{\text{DSP}}|(T, p) = \Omega\gamma\sigma_0^2/(6m_0T \ln L)$, such that the SD (MD) regime holds for $|h| < |h_{\text{DSP}}|$ ($|h| > |h_{\text{DSP}}|$).

We measured τ in MC simulations using rejection-free methods [17, 18]. This is in Fig. 4 together with our predictions. Interesting enough, we observe that τ increases with T for fixed $p > 0$ at low- T . That is, the local stability of *nonequilibrium* metastable states is enhanced by the addition of thermal noise. This behavior resembles the noise-enhanced stability (NES) phenomenon reported in experiments on unstable systems [19], which is in contrast with the simple Arrhenius law observed in equilibrium. Remarkably, only *thermal* NES is observed: Increasing p for fixed T always results in shorter τ . This complex phenomenology is captured by our simple ansatz, which traces back the NES phenomenon to the low- T anomaly in σ_0 . More generally, the stochastic resonance in τ (and v_0) stems from a nonlinear co-operative interplay between thermal and nonequilibrium noises. Although both noise sources induce disorder when applied independently, their combined effect results in a resonant stabilization of the metastable phase at low- T . This non-linear effect is also reflected in the morphology of the metastable-stable transition. In particular, $|h_{\text{DSP}}|$ inherits the non-monotonous T -dependence of σ_0 , see top inset to Fig. 4, resulting in a novel MD regime at low- T not observed in equilibrium. This is confirmed by direct inspection of escape configurations, e.g. Fig. 1.

One may get further physical insight by rewriting the rate (1) as $p + (1 - p)\Psi(x_i) \equiv \Psi(x_i^{\text{ef}})$, with $x_i = \beta\Delta\mathcal{H}_i$ and $x_i^{\text{ef}} = \beta_{\text{ef}}\Delta\mathcal{H}_i$. The resulting effective temperature $T_{\text{ef}}(x_i, p) \equiv \beta_{\text{ef}}^{-1}$ then follows as $T_{\text{ef}}/T =$

$x_i (x_i + \ln[(1-p)/(1+pe^{x_i})])^{-1}$. For any $p > 0$, T_{ef} changes from spin to spin and depends on the *local order* (e.g. number of broken bonds for a given spin): the smaller the number of broken bonds, the higher the local order, and the larger the effective temperature. Therefore, for $p > 0$, the strength of fluctuations affecting a spin increases with the local order parameter. This is the fingerprint of *multiplicative noise*, and it allows us to write a Langevin equation which captures the essential physics. In its simplest, 0-dimensional form, this equation is $\partial_t \psi = \psi - \psi^3 + h + \sqrt{D + \mu \psi^2} \xi(t)$, where $\xi(t)$ is a Gaussian white noise with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t) \xi(t') \rangle = 2\delta(t - t')$, D is the strength of the thermal noise, h is a magnetic field, and μ is the renormalized version of the nonequilibrium parameter p . This equation describes a *Brownian particle* in an asymmetric bimodal potential, $V(\psi) = -\frac{1}{2}\psi^2 + \frac{1}{4}\psi^4 - h\psi$, subject to fluctuations which increase with ψ^2 and whose amplitude remains non-zero as $D \rightarrow 0$ for any $\mu > 0$ [17]. A full description of the problem, including the compact excitations observed in simulations, would of course involve the spatially-extended version of this equation. However, the above toy mean-field equation already contains the essential competition between thermal (D) and nonequilibrium (μ) fluctuations in a metastable potential which characterizes our system. The steady distribution of the stochastically-equivalent Fokker-Planck equation in Stratonovich sense is $P_{\text{st}}(\psi) = \Lambda[2\sqrt{\mu(D + \mu\psi^2)}]^{-1} \exp[-D^{-1}W(\psi)]$, where $W(\psi) = \frac{d}{2}[\psi^2 - (1+d)\ln(d + \psi^2)] - hd^{1/2} \tan^{-1}(\psi d^{-1/2})$, with $d \equiv D/\mu$ and Λ a normalization constant. The extrema of the effective potential $W(\psi)$ are the same than those of $V(\psi)$, namely $\psi_k = 2\cos(\theta_k)/\sqrt{3}$, with $\theta_k = \frac{1}{3}[\cos^{-1}(-\frac{1}{2}\sqrt{27}h) + 2k\pi]$, and $k = 0, 1, 2$. For $h < 0$, ψ_0 , ψ_1 and ψ_2 correspond to the metastable, stable and unstable extrema, respectively, and the escape time from the metastable minimum is $\tau(D, \mu, h) \approx 2\pi[|V''(\psi_0)V''(\psi_2)|]^{-1/2} \exp[\frac{1}{D}(W(\psi_2) - W(\psi_0))]$, where $V'' = \partial_x^2 V(x)$. Identifying D with temperature, this approach recovers the thermal NES phenomenon for τ observed in the microscopic model (see bottom inset to Fig. 4).

Summing up, we have shown that introducing a nonequilibrium condition has important effects on metastable dynamics. The non-linear interplay between thermal and nonequilibrium fluctuations, as captured by σ_0 , results in resonant low- T phenomena, e.g., noise-enhanced stabilization of the metastable state and resonant domain wall propagation, that are not observed in equilibrium, but are likely to characterize a broad class of actual systems dominated by dynamic impuri-

ties. Surprisingly, these far-from-equilibrium phenomena can be understood using nucleation theory, based on a nonequilibrium potential at a mesoscopic/cluster level. This is possible because the relevant excitations driving the metastable-stable transition result from a competition between a surface and a bulk. This suggests that our approach may prove useful for studying metastability in many other nonequilibrium systems where a surface-bulk competition plays a significant role.

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